

Atomic data: EPICS2014

*D. Brown
for Red Cullen*



Coupled photon-electron data used in radiation shielding applications

- **For use in Shielding Applications we need**
 - Photon Interaction Data
 - including direct secondary photons and electrons
 - Electron Interaction Data
 - including direct secondary photons and electrons
- **Data for ALL Photon-Electron Coupling**
 - Fluorescence X-Rays and Auger Electrons
- **Computer Codes to Use This data**
 - Using Accurate Radiation Transport Methods
 - Monte Carlo
 - Data is Useless without Codes
 - Codes are Useless without Data



INTERNATIONAL ATOMIC ENERGY AGENCY

NUCLEAR DATA SERVICES

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**EPICS2014:
Electron Photon Interaction Cross Sections
(Version 2014)**

by

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Abstract: EPICS2014 is the Electron Photon Interaction Cross Section library that provides the atomic data needed to perform coupled Electron-Photon transport calculations, to produce accurate macroscopic results, such as energy deposition and dose. Atomic data is provided for elements, $Z = 1$ to 100, over the energy range 10 eV to 100 GeV; nuclear data, such as photo-

EPICS2014 consists of 4 libraries

- ***The Evaluated Electron Data Library (EEDL)***, to describe the interaction of electrons with matter.
- ***The Evaluated Photon Data Library (EPDL)***, to describe the interaction of photons with matter.
- ***The Evaluated Atomic Data Library (EADL)***, to describe the emission of electrons and photons back to neutrality following an ionizing event, caused by either electron or photon interactions
- ***The Evaluated Excitation Data Library (EXDL)***, to describe the excitation of atoms due to photon interaction

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- ***The Evaluated Neutron Data Library (ENDL)***, to describe the interaction

In ENDF & ENDL formats

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ba
ca

In ENDL format only

- *The Evaluated Excitation Data Library (EXDL)*, to describe the excitation of atoms due to photon interaction

ENDF Photo-atomic library has a long history

Designation	Date	ENDF/B Version	Comments
DLC-7/ HPICE	Sep. 1969		Initial release
DLC-7C/ HPICE	Jan. 1970	ENDF/B-II	Named ENDF/B-II photon interaction library
DLC-7D/ HPICE	Apr. 1971	ENDF/B-III	Pair production increased by 3-5%; incoherent scat. corrected 0.8 MeV for Z=31-34
DLC-7E/ HPICE	July 1975	ENDF/B-IV	File 27 data added & replaced file 23 cross sections
DLC-7F/ HPICE	Oct. 1975	ENDF/B-IV	Update previous data with new 1973 Fundamental Constants
DLC-99/ HUGO	Dec. 1983	ENDF/B-V	Updated with new National Bureau of Standards data; new ENDF/B-V format

see Roussin, et al. ENDF-335 (1983)

In 1990, ENDF/B-VI.0 expanded atomic data to include electrons and atomic relaxation

- **Based on S. Perkins & Red Cullen's EPDL**
 - UCRL-50400 Vol. 6 Rev. 4 (1989)
 - photons from 10 eV — 100 GeV
- **Revised in 1997**
 - photons extended down to 1 eV, add photoionization to compute anomalous scattering factors, photo-excitation data
- **Major upgrade in 2001: atomic relaxation (EADL) & electrons (EEDL)**
 - UCRL-50400 Vol. 31 (1991) — EEDL
 - UCRL-50400 Vol. 30 (2001) — EADL
 - Electron data translated to ENDF by R. MacFarlane

EPICS2014

- **Major changes:**

- Corrected incorrectly translated electron data (MF/MT=26/527, $\langle E \rangle$ from Bremstrahlung)
- Increase file precision with ENDF2C
- “Changes where I felt they were necessary”

- **Major change not made:**

- Revising transition energies to match results of Deslattes, et al., “X-ray transition energies: a new approach to a comprehensive evaluation”, Rev. Mod. Phys. **75**, 35-99 (2003).
- Used for validation (see next slides)

- **Update seems minor, but important to upgrade all sub libraries as a set to maintain internal consistency**

Comparison to Rev. Mod. Phys. eval.

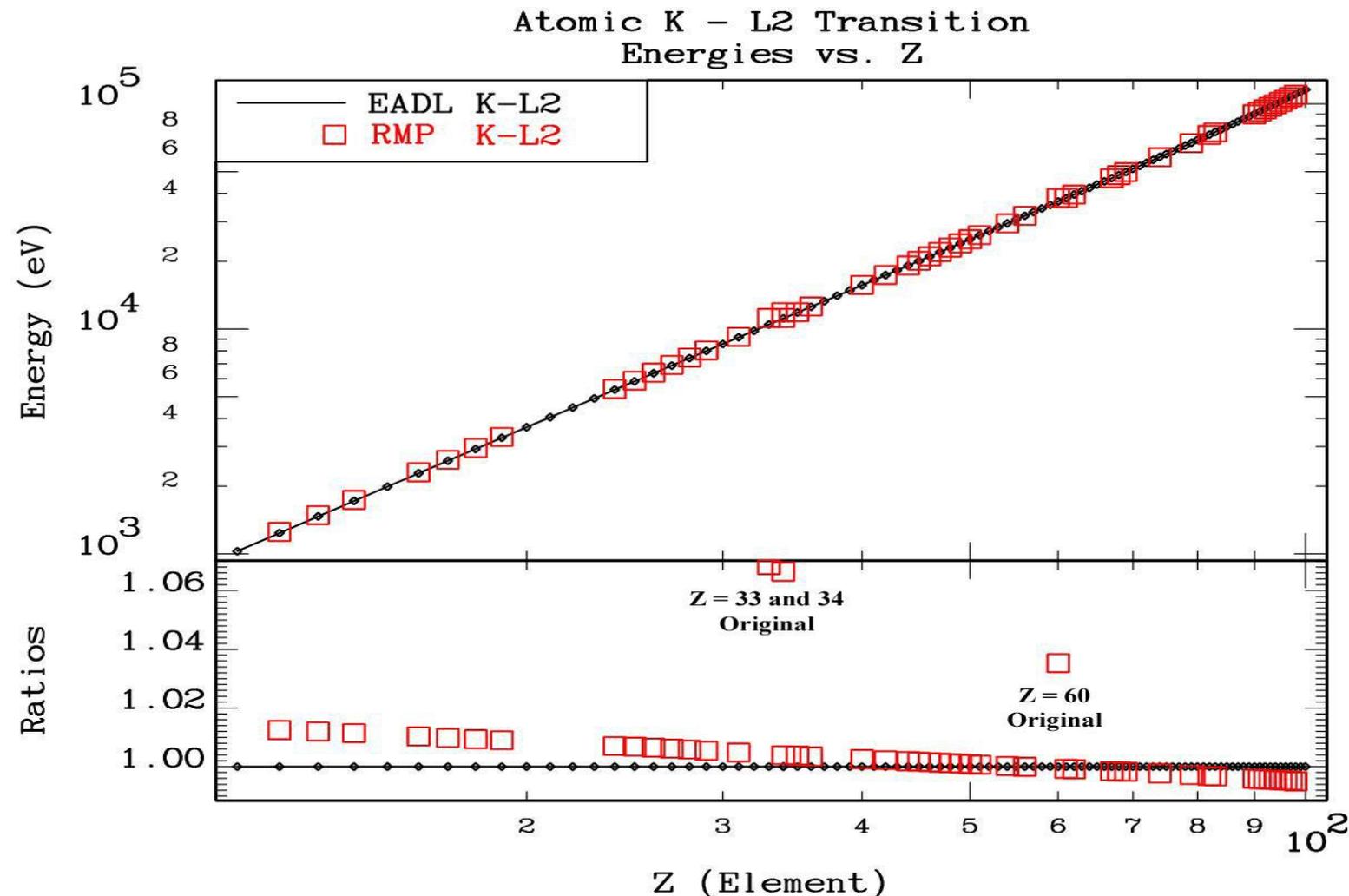


Fig. 1: Comparison of Original K - L2 Transition Energies

Rev. Mod. Phys. eval. fixed

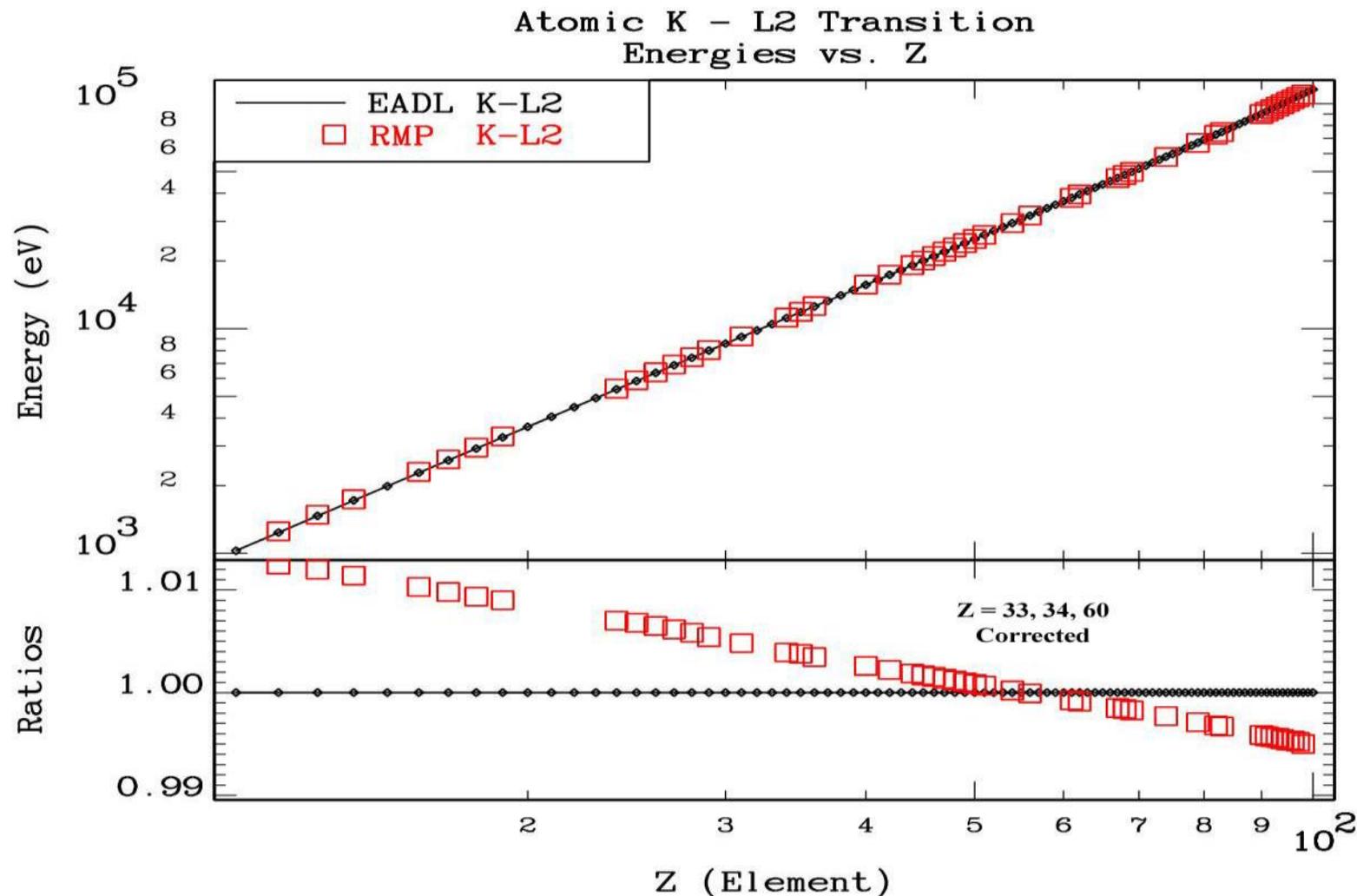
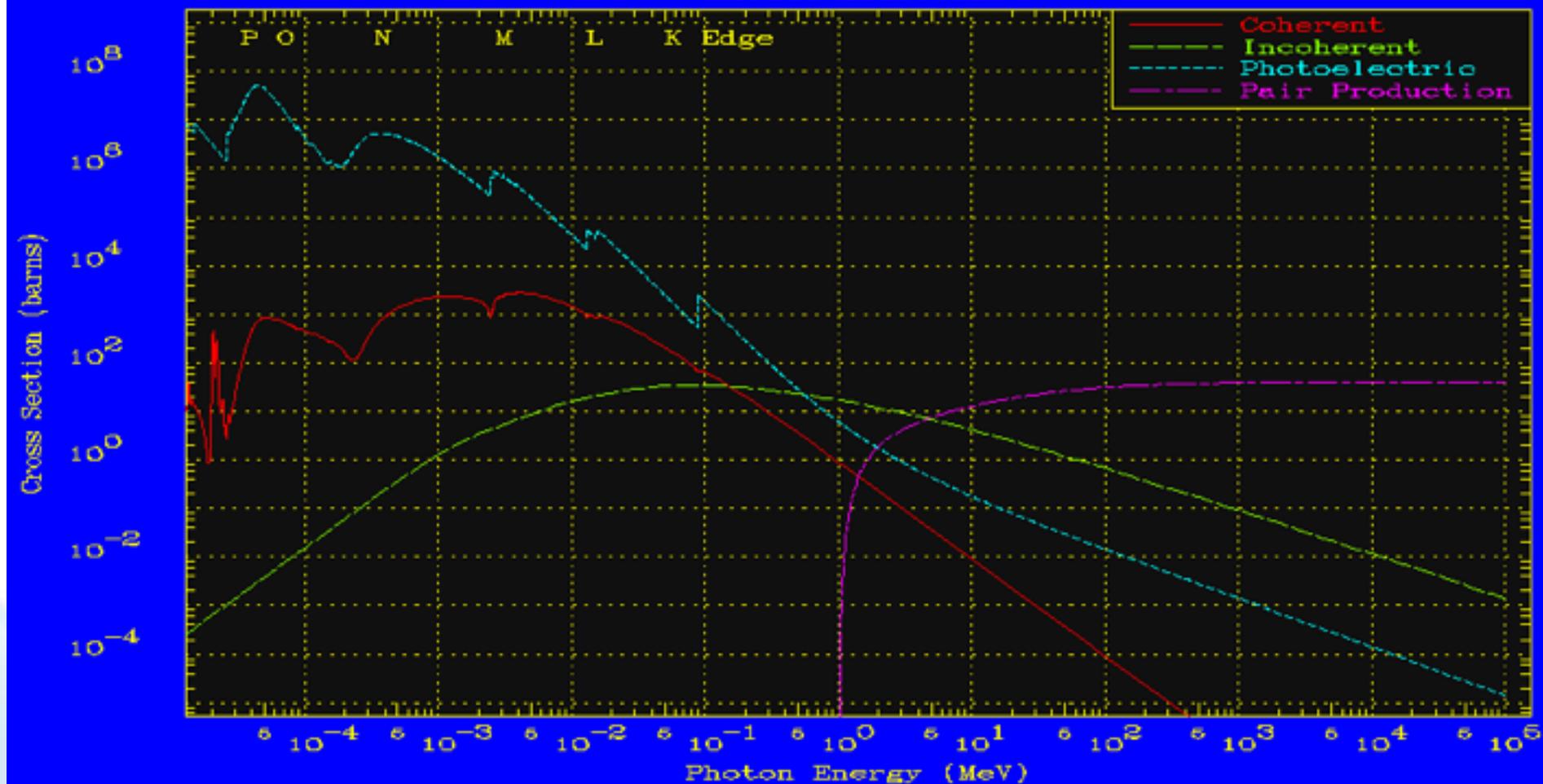


Fig. 3: Comparison of Corrected K - L2 Transition Energies

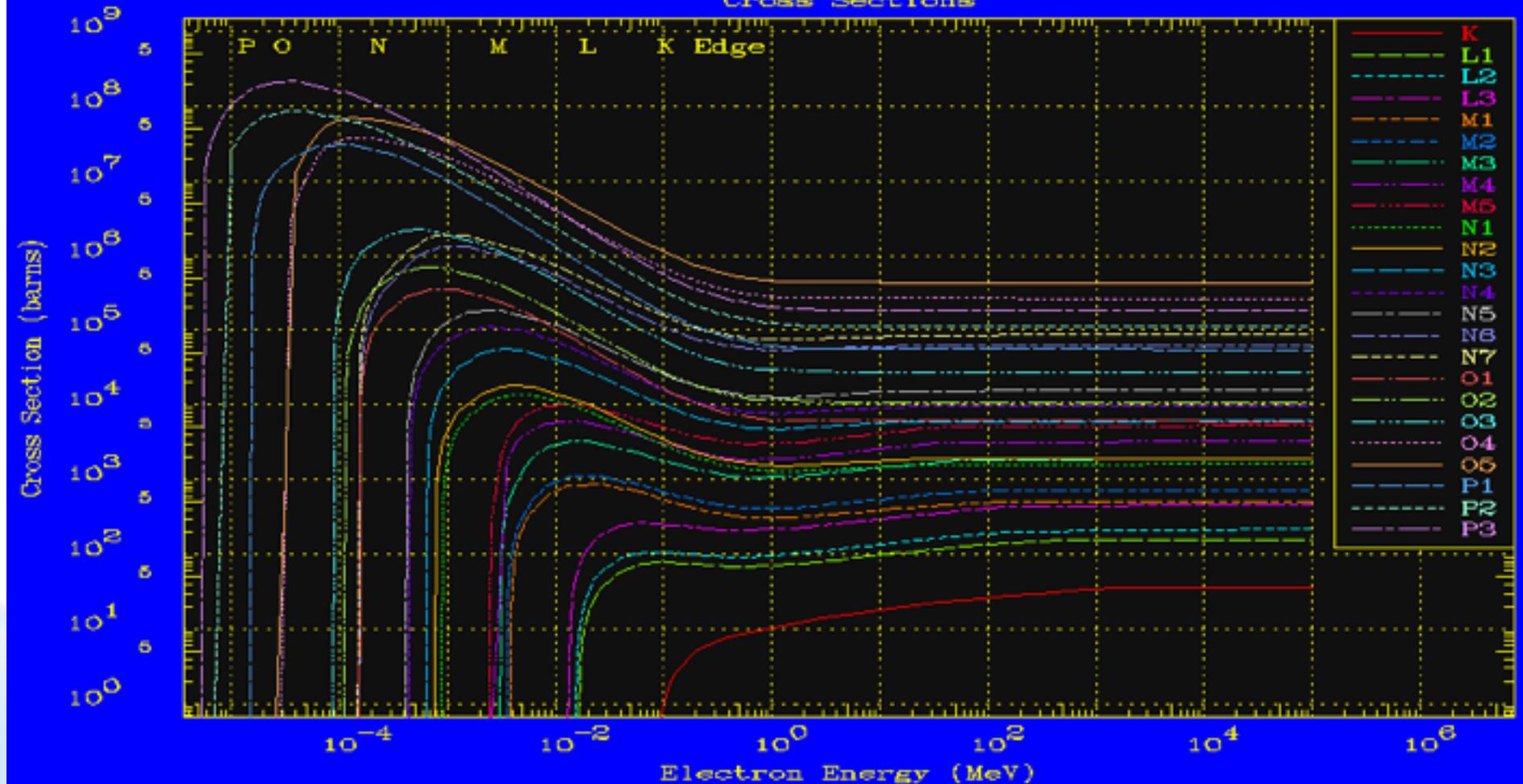
Typical photon cross sections

Figure 1: Lead Photon Interaction Cross Sections



Typical electron ionization cross sections

Figure 3: Lead Electron Ionization Cross Sections



Although updating library makes sense, we do need to be able to test it

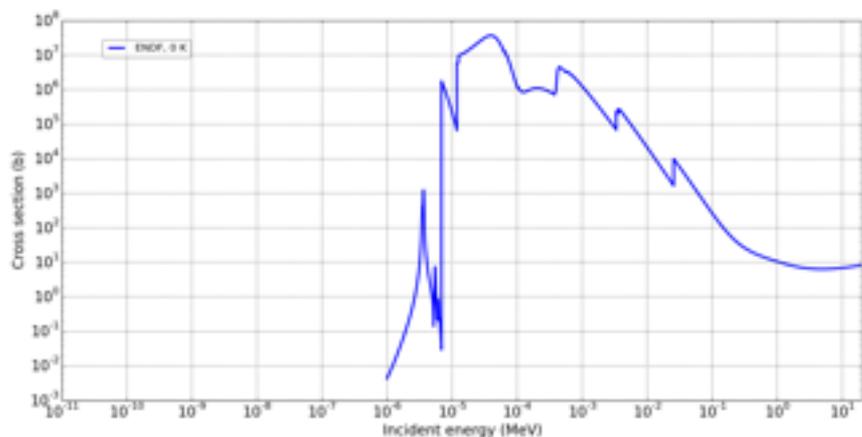
- **B. Beck added capability to read photo-atomic and electro-atomic data in Fudge**
 - This includes simple physics checks
- **D. Brown added plotting capabilities for this data in Fudge**
 - This includes cross sections, form factors and anomalous scattering functions
- **Fudge, PREPRO and NNDC checking codes now can check atomic data automatically with ADVANCE**

What's in the photo-atomic sub library?

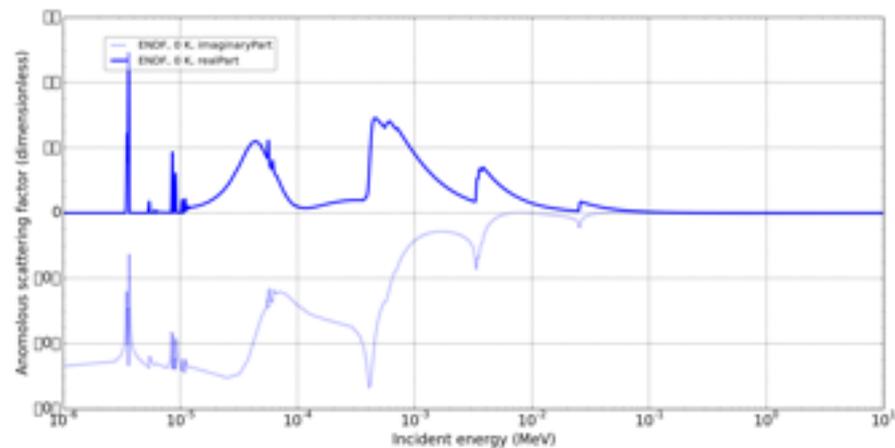
- **Coherent scattering,**
 - *integrated cross section (b),*
 - *form factor,*
 - *real and imaginary anomalous scattering factors,*
 - average energy of the scattered photon (MeV),
- **Incoherent scattering**
 - *integrated cross section (b),*
 - *scattering function,*
 - average energy of the scattered photon and recoil electron (MeV).
- **Total photoelectric reaction**
 - *integrated cross section (b),*
 - average energy to the residual atom, i.e., local deposition (MeV),
 - average energy of the secondary photons and electrons (MeV).
- **Photoelectric reaction, by subshell**
 - *integrated cross section (b),*
 - average energy to the residual atom, i.e., local deposition (MeV),
 - average energy of the secondary photons and electrons (MeV) .
- **Pair production reaction**
 - *integrated cross section (b),*
 - average energy of the secondary electron and positron (MeV) .
- **Triplet production reaction**
 - *integrated cross section (b),*
 - average energy of the secondary electron and positron (MeV) .

green == ADVANCE can plot

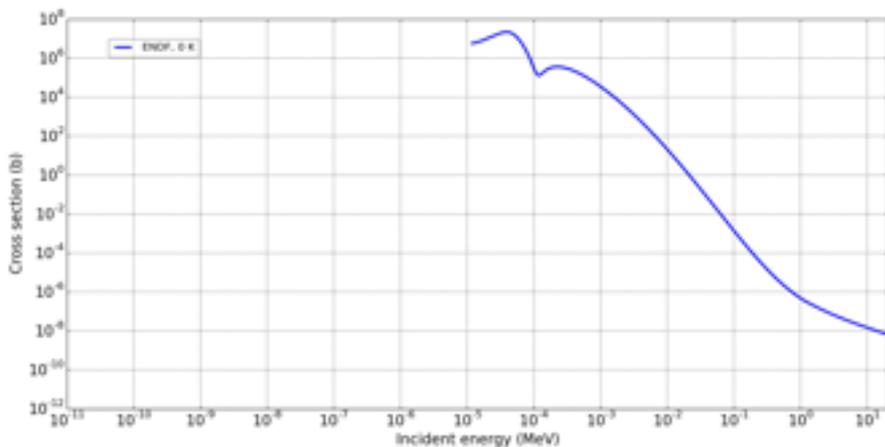
gamma+Ag, Total photon interaction (MT=501)



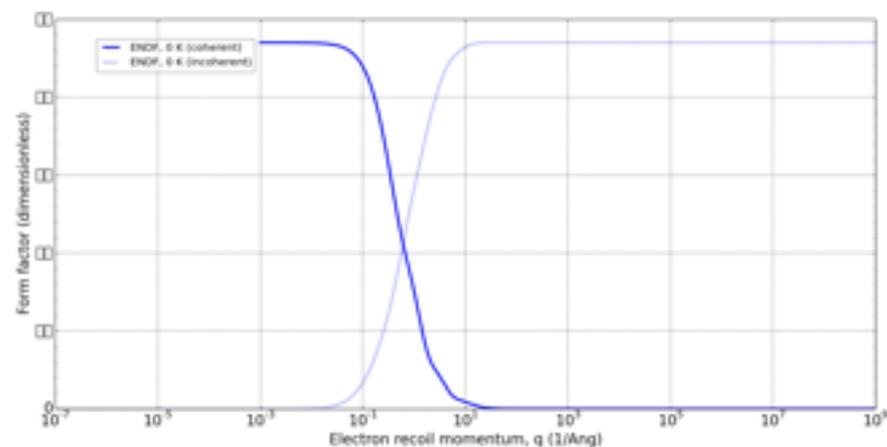
gamma+Ag, Photon coherent scattering (MT=502), anomalous scattering factor



gamma+Ag, N5 shell ionization (MT=547)



gamma+Ag, Photon (in)coherent scattering form factors (MT=502,504)

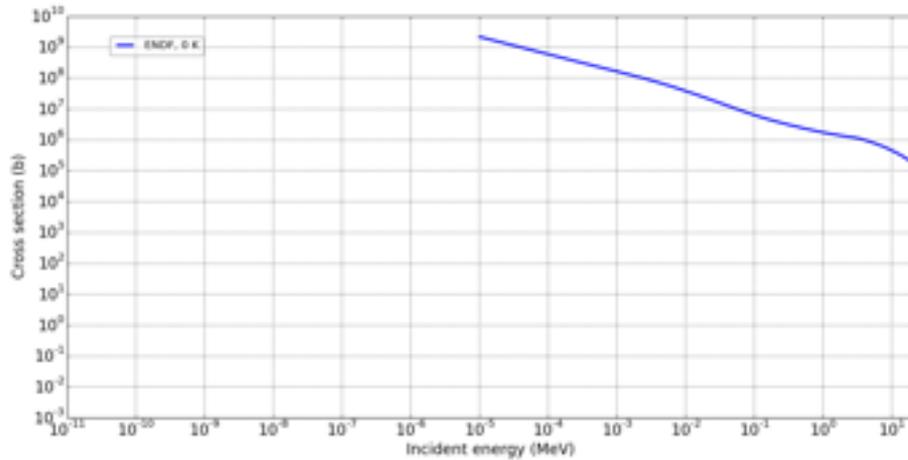


What's in the electro-atomic sub library?

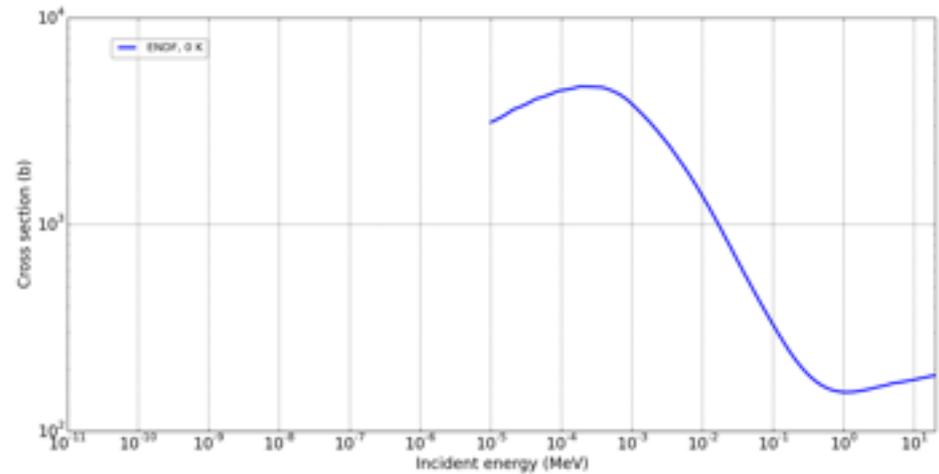
- Elastic transport,
 - *transport cross section, σ_{el} ($1-E\langle\cos\theta\rangle$) (b)*
- Large angle elastic scattering (over $\cos\theta = -1$ to 0.999999)
 - *integrated LACS cross section (b),*
 - average energy of the scattered electron (MeV),
 - average energy to the residual atom, i.e., local deposition (MeV),
 - angular distribution of the scattered electron.
- Elastic scattering
 - *integrated scattering cross section (b),*
- Ionization, by subshell
 - *integrated cross section (b),*
 - average energy to the scattered and recoil electron (MeV)
 - spectra of the recoil electron (MeV^{-1}).
- Bremsstrahlung
 - *integrated cross section (b),*
 - average energy of the secondary electron and photon (MeV) ,
 - spectra of the secondary photon (MeV^{-1}).
- Excitation
 - *integrated cross section (b),*
 - average energy to the residual atom, i.e., local deposition (MeV).

green == ADVANCE can plot

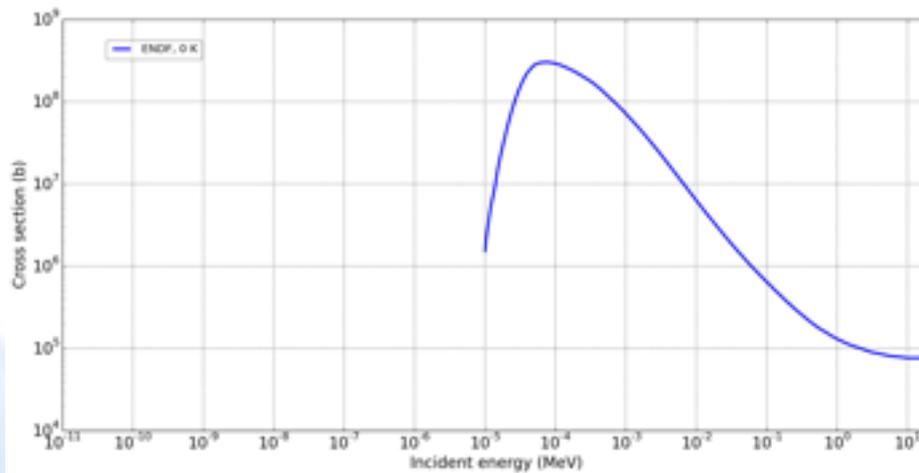
e+Co, Electro-atomic scattering (MT=526)



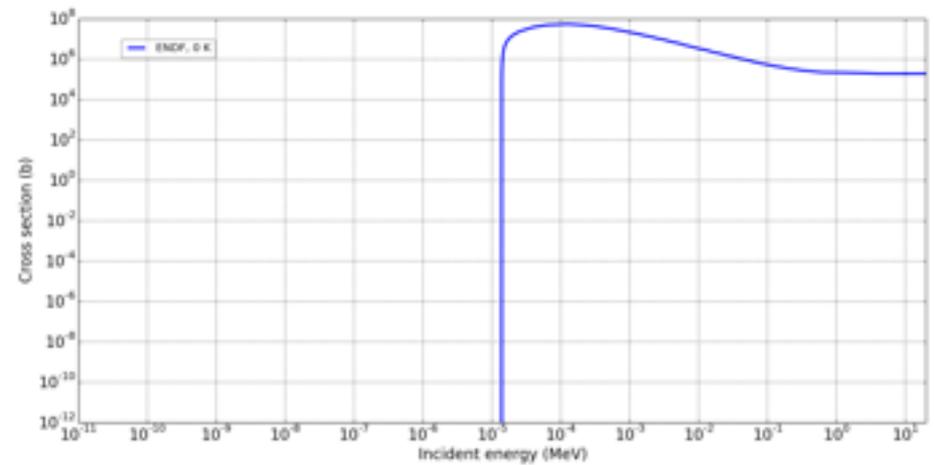
e+Co, Bremstrahlung (MT=527)



e+Co, Electro-atomic excitation (MT=528)



e+Co, M4 shell ionization (MT=541)



What's in the atomic relaxation sub library?

■ Subshell data

- number of electrons,
- binding and kinetic energy (MeV),
- average radius (cm),
- radiative and nonradiative level widths (MeV),
- average number of released electrons and x-rays,
- average energy of released electrons and x-rays (MeV),
- average energy to the residual atom, i.e., local deposition (MeV).

■ Transition probability data

- radiation transition probabilities,
- nonradiative transition probabilities.

What parts of this data can we test? How can we test this data?

Who uses is this data in practice?

- **LLNL currently uses data in original ENDL format**
 - ENDL formatted data used in ASC codes
 - Fudge can read ENDF photon and electron data, plot it & do some checks, but not used in production environment
 - COG uses EGS
- **LANL processes with NJOY**
 - We could not replicate the photo-atomic file processing of ENDF/B-VII.1 distributed with MCNP
 - Rumored that required significant hand edits
- **BNL uses only atomic relaxation library when producing Decay sub library**
- **Data integrated into EGS package and used in many other code systems**